Title: **Development of Nanofiller-Modulated Polymeric Oxygen Enrichment Membranes for Reduction of Nitrogen Oxides in Coal Combustion**

Author(s): Dr. Jianzhong Lou (PI)
Dr. Shamsuddin Ilias (Co-PI)
Department of Mechanical and Chemical Engineering
North Carolina A&T State University
1601 E. Market St.
Greensboro, NC 27411
Phone: (336) 334-7620
FAX: (336) 334-7417
E-mail: lou@ncat.edu
Grant Number DE-FG26-06NT42742
Performance Period 2/17/06 – 2/16/09

OBJECTIVE(s)

The major objectives are: (1) Develop a polymer material that incorporates functional nanofillers to achieve novel oxygen-enrichment permselectivity; (2) Document the fundamental microstructure-property relationship of the nanofiller-modulated polymer material using molecular simulation.

ACCOMPLISHMENTS TO DATE

The influence of nanofillers on the self diffusion, free volume, glass transition and in turn the oxygen diffusion and solubility and the permselectivity of oxygen in polymer membrane is studied. Thermal properties were investigated by experiments and molecular dynamics simulations. Molecular models of Single-walled carbon nanotubes PDMS membrane and nano fumed silica PDMS membrane, zeolite-modulated polyimide membrane were built by Material Studio 4.0 and the resulting output coordinate files were modified to make them compatible with GROMACS. All Molecular dynamics simulations were performed using the GROMACS 3.3 simulation package on a 40-node IBM xSeries Linux Cluster. Modified OPLS-AA force field was used. In the simulations, the leapfrog algorithm was used to integrate Newton's equations of motion with a time step of 2 fs. Periodic boundary conditions were applied and nonbonded force calculations employed a grid system for neighbor searching. In this system, only the atoms in the neighboring grid cells are considered when building a new neighbor list. A twin-range cutoff was used for both Lennard-Jones and Coulombic calculations. The permeation and diffusion experiments were performed for the different membranes with different amount of nanofillers.

FUTURE WORK

A number of polysiloxanes, polyimides are being studied for gas separation with the selective incorporation of various nanofillers including surface modified carbon nanotubes, surface modified silica nanoparticles, and various molecular sieves. The mechanisms are studied by molecular simulation regarding the diffusion and the solubility of oxygen in the polymer which is modulated by these nanofillers.

LIST OF PAPER PUBLISHED

1. J. Zhang, J. Lou, S. Ilias, P. Krishnamachari, J. Yan. "Thermal properties of poly(lactic acid) fumed silica nanocomposites: Experiments and molecular dynamics simulations", Polymer, **2008** 49, 2381-2386.
2. J. Zhang, Y. Liang, J. Yan, **J. Lou**, "Study of molecular weight dependence of glass transition temperature for amorphous poly(l-lactide) by molecular dynamics simulation", Polymer. **2007** 48, 4900-4905.

U.S. PATENT/PATENT APPLICATION(S) n/a

CONFERENCE PRESENTATIONS n/a

AWARDS RECEIVED AS A RESULT OF SUPPORTED RESEARCH n/a

STUDENTS SUPPORTED UNDER THIS GRANT James Zhang – PhD candidate